Degree of crosslinking in combustion carbons

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In this work, we estimated the degree of crosslinking within mature soot particles making use of reactive force field molecular dynamics (MD) simulations to determine the mechanical properties of crosslinked polycyclic aromatic hydrocarbons (PAHs).

PAHs are essential components of carbonaceous nanoparticles formed in combustion processes. These particles present a pressing problem to human health and the climate, but can also produce many novel carbon materials used as pigments, reinforcing rubbers and battery anodes. The transition from the gas phase to the condensed phase leads to carbonaceous particle - also known as soot - in combustion processes is poorly understood. Therefore, understanding their degree of crosslinking is important for determining which mechanisms and precursors are involved in their inception and growth.

Nanoindentation reactive force field MD simulations of carbonaceous nanoparticles of crosslinked aromatic molecules have been made. Forty-two model nanoparticles with different sizes and degrees of crosslinking were built. The hardness, elastic constant and Poisson's ratio of each particle were calculated and the results were compared with nanoindentation experiments of soot particles in order to understand how these properties are related to the degree of crosslinking in these particles. The results show that mature soot particles are expected to present crosslinks between their aromatic constituents to have a comparable value of the hardness found experimentally.

These results provide valuable information on soot morphology and formation mechanism, revealing the importance of crosslinking reactions during soot maturation that give rise to a structure in which the majority of aromatics are aliphatically-linked.